

### **3. CHEMICAL AND PHYSICAL INFORMATION**

#### **3.1 CHEMICAL IDENTITY**

Ethylbenzene is an aromatic hydrocarbon that occurs naturally in petroleum and is a component of aviation and automotive fuels. It is used as a solvent and in the production of synthetic rubber and styrene.

Information regarding the chemical identity of ethylbenzene is located in Table 3- 1.

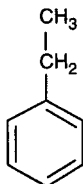
#### **3.2 PHYSICAL AND CHEMICAL PROPERTIES**

Ethylbenzene is a colorless liquid with an aromatic odor. Information regarding the physical and chemical properties of ethylbenzene is located in Table 3-2. Ethylbenzene is a flammable and combustible liquid.

Vapors are heavier than air and may travel to a source of ignition and flash back. Liquid ethylbenzene floats on water and may travel to a source of ignition and spread fire. Combustion may produce irritants and toxic gases (NFPA 1994). Ethylbenzene may accumulate static electricity and will react with oxidizing materials (NFPA 1994).

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**Table 3-1. Chemical Identity of Ethylbenzene**

Characteristic	Value	Reference
Chemical name	Ethylbenzene	Merck 1989
Synonyms	EB; ethyl benzene; ethylbenzol; phenylethane	HSDB 1995
Trade names	No data	
Chemical formula	C <sub>8</sub> H <sub>10</sub>	Merck 1989
Chemical structure		
Identification numbers:		
CAS Registry	100-41-4	Merck 1989
NIOSH RTECS	NIOSH/DAO700000	HSDB 1995
EPA Hazardous Waste	F003; Ethylbenzene	HSDB 1995
OHM/TADS	7216709	HSDB 1995
DOT/UN/NA/IMCO	UN 1175; Ethylbenzene	HSDB 1995
Shipping	IMO 3.2, Ethylbenzene	HSDB 1995
HSDB	84	HSDB 1995
NCI	NCI-C56393	HSDB 1995
STCC	49 091 63; Ethylbenzene	HSDB 1995

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Databank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances; STCC = Standard Transport Commodity Code

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**Table 3-2. Physical and Chemical Properties of Ethylbenzene**

Property	Values	References
Molecular weight	106.17	Lide 1994
Color	Colorless	Merck 1989
Physical state	Liquid	Merck 1989
Melting point	-95 °C	Lide 1994
Boiling point	136.2 °C	Lide 1994
Density at 20 °C/4 °C	0.8670	Lide 1994
at 25 °C/25 °C	0.866	Merck 1989
Odor	Sweet, gasoline-like	CHRIS 1985
Odor threshold:		
Water	0.029 mg/L 0.140 mg/L	Amoore and Hautala 1983 Rosen et al. 1963; Verschueren 1983
Air	2.3 ppm 2–2.6 mg/m <sup>3</sup>	Amoore and Hautala 1983 Verschueren 1983
Solubility:		
Water at 0 °C	197 mg/L	Polak and Lu 1973
at 15 °C	140 mg/L	Verschueren 1983
at 20 °C	152 mg/L	Verschueren 1983
at 25 °C	160 mg/L	Amoore and Hautala 1983
at 25 °C	177 mg/L	Polak and Lu 1973
at 25 °C	208 mg/L	Bohon and Claussen 1951
Organic solvents	Miscible with usual organic solvents Soluble in alcohol and ether	Merck 1989 Lide 1994
Partition coefficients:		
Log K <sub>ow</sub>	4.34 3.13 3.15	Mabey et al. 1982 Yalkowsky and Valvani 1976 Hansch and Leo 1979
Log K <sub>oc</sub>	2.22 (calculated) 2.38 (measured) 2.40 (calculated)	Chiou et al. 1983 Hodson and Williams 1988 Vowles and Mantoura 1987
Vapor pressure		
at 20 °C	7 mm Hg	Verschueren 1983
at 25 °C	1.27 kPa (9.53 mm Hg)	Mackay and Shiu 1981
at 25.9 °C	10 mm Hg	Sax and Lewis 1989
at 30 °C	12 mm Hg	Verschueren 1983
at 74.1 °C	100 mm Hg	OHM/TADS 1988
Henry's law constant:		
at 20 °C	6.6x10 <sup>-3</sup> atm-m <sup>3</sup> /mol	Mabey et al. 1982
at 20 °C	8.7x10 <sup>-3</sup> atm-m <sup>3</sup> /mol	Lyman et al. 1982
at 25 °C	8.43x10 <sup>-3</sup> atm-m <sup>3</sup> /mol	Mackay et al. 1979
at 25 °C	7.9x10 <sup>-3</sup> atm-m <sup>3</sup> /mol	Mackay and Shiu 1981
Autoignition temperature	810°F (432°C)	NFPA 1994
Flash point	70°F (21°C)	NFPA 1994
Flammability limits	0.8 (lower) vol% – 6.7 (upper)vol%	NFPA 1994
Conversion factors	1 mg/m <sup>3</sup> = 0.23 ppm 1 ppm = 4.35 mg/m <sup>3</sup>	Verschueren 1983

